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Equations were derived which rigorously codify the propagation of fields in finite-difference time-domain (FDTD) grids. These equations were then used to construct a perfect total-field/scattered field boundary (which is used to inject energy into the grid).							
Algorithms were developed to enhance the modeling of material boundaries in the FDTD method; the accuracy of various FDTD or							
FDTD-like algorithms were rigorously studied; an FDTD algorithm was developed which is theoretically exact (i.e., provided the							
grid is infinite the accuracy is limited only by the finite precision of computers); various computer programs related to the FDTD							
method were written; and information and programs were disseminated via journal publications, conference presentations, and the Web.							
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## Final Report: Numerical Studies of Acoustic Propagation in Shallow Water

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The FDTD method is obtained by discretizing the differential equations that govern the underlying system. Using a Cartesian grid, the method provides an exceedingly simple way in which to express future fields (i.e., unknown fields) in terms of past fields (known fields). For propagation in a homogeneous region, the traditional FDTD method is accurate to second-order—that is, doubling the number of grid points per wavelength reduces inherent numerical errors by a factor of four.

The behavior of fields and accuracy of the FDTD method at material interfaces are much more complicated than in a homogeneous region. We previously derived exact expressions describing the behavior of plane waves at planar boundaries [1,2]. Additionally we have examined and developed ways to minimize the errors associated with the "stairstep approximation" which is inherent when modeling continuously varying surfaces in the FDTD method [3-8]. The work most recently published in The Journal of the Acoustical Society of America showed how employing a simple modification of the equations used to updated the fields adjacent to a rigid boundary could significantly improve the accuracy of the simulation [8].

We continued to explore several new implementations of the FDTD method (proposed by others) which seek to minimize dispersive and anisotropic errors inherent in all 2- and 3-D FDTD schemes. Our comparisons provide insight into the techniques that are not easily garnered from the publications in which they were originally presented. Some of this work appeared in IEEE Transactions on Microwave Theory and Techniques [9] and was presented at the 2002 URSI/Antennas and Propagation Symposium [10]. Notably, we demonstrated that many of the wavelet-based schemes, which have attracted some advocates, are not superior to an FDTD scheme that uses the same spatial stencil and the same "computational effort" (i.e., operations per a given temporal advancement of the fields). We have further expanded on this work in a recent publication [11].

Our investigations of the discretized worlds of FDTD methods have led us to a better understanding of numeric artifacts associated with resonances and to ways of alleviating these artifacts. Part of this work was presented as an invited talk in a special session organized by Prof. Allen Taflove (one of the co-founders of the FDTD method) [12]. This work is further described in a paper which has recently appeared in IEEE Transactions on Antennas and Propagation [13]. In that work we show how the anisotropic dispersion inherent in the traditional "Yee" FDTD algorithm can cause rather bizarre behavior in the resonant modes of a canonical resonator. Modes which are degenerate in the continuous (or "real") world can split into multiple modes. On the other hand, modes which are distinct in the continuous world may be degenerate in the discrete FDTD world. Additionally, even modes that are not split or recombined in some spurious manner in the FDTD world can nevertheless be shifted from the true resonant frequency that pertains in the continuous world. Our work provides a way to quantify this behavior exactly without ever needing to perform an FDTD simulation.

Given this understanding of the traditional FDTD technique, we were motivated to explore a technique which was more isotropic than the traditional FDTD technique. Thus, we developed a variation of the promising FDTD scheme proposed by Eric Forgy (*IEEE Transactions on Antennas and Propagation*, **50**(7):983–996, 2002). This algorithm suffers much less grid dispersion and anisotropy than more traditional FDTD formulations but still retains the local nature of the standard update equations. The acoustic implementation of this algorithm is described in a paper was published in the *Journal of Computational Acoustics* [14].

A recent publication by John Pendry (Phys. Rev. Lett., 85:3966, 2000) which described the use of backward-wave (BW) materials to make a "perfect lens" has received considerable attention. BW materials are dispersive materials whose direction of phase propagation is antiparallel to the direction of power flow. BW materials can exist in both acoustic and electromagnetic systems. BW materials belong to the class of materials know as "metamaterials" since they do not occur in nature (i.e., they must be manufactured). There is great interest in metamaterials since they can have interesting and useful properties not found in natural materials. Our initial attempts to model BW materials using the FDTD technique were not consistent with those one would expect from an initial inspection of the theory. Eventually we discovered that the dual, offset grids employed in the FDTD method (i.e., the dual pressure and velocity grids or the dual electric and magnetic field grids) can introduce significant numeric artifacts when modeling BW materials. The offset in the grids can introduce a boundary layer that has the material properties of neither the BW material nor the surrounding medium. Our investigations were presented in an invited talk at the 2002 URSI/Antennas and Propagation Symposium [15] and in a paper which was published in Physical Review Letters B [16]. These publications focused on the behavior of fields in the continuous world when a BW material has a small boundary layer. A recent publication in *IEEE Transactions* on Antennas and Propagation described specific implementation issues concerned with modeling BW materials using the FDTD method [17]. It was shown that the Pseudospectral Time-Domain (PSTD) method, which employs a collocated grid and uses discrete Fourier transforms to calculate spatial derivatives, may provide superior results to the FDTD method when modeling these materials.

The Yee FDTD algorithm can provide exact solutions to one-dimensional problems when operated at the so-called magic time step (i.e., when the spatial step size is equal to the speed of light times the temporal step size). Here "exact" is taken to mean the field propagates without dispersion error or other numeric artifacts beyond those which are dictated by the finite precision of the computer. Unfortunately there is no magic time step in higher dimensions. However we have recently developed a theoretical framework for multi-dimensional algorithms that have the same exact properties as the one-dimensional Yee algorithm when operated at a particular time step. The proposed technique uses vector operators which, instead of being defined at a point such as with the usual gradient, divergence, and curl operators, are defined over spheres. Due to their inherent symmetry, these spatial operators have the same properties in all directions. With

a judicious choice of the temporal step size the temporal errors can cancel the spatial errors and the algorithm is exact. However, although the framework for the algorithm has been developed, no practical (i.e., computationally efficient) algorithm has yet been developed. It should also be noted that the method is only theoretically exact on an infinite grid—a finite grid will introduce some inherent error but that error will be smaller than traditional FDTD techniques. Nevertheless proof-of-concept implementations of the algorithm (which are quite computationally expensive) have been used to demonstrate the validity of the technique and the improvements the algorithm can provide over other FDTD implementations. The algorithm also has interesting properties such as unconditional stability for an arbitrary temporal step size. Some of our work on this algorithm was presented as an invited talk at the 2003 URSI/Antennas and Propagation Symposium [18]. This work is further described in a publication in *Journal of Computational Physics* [19] and a Ph.D. dissertation (the author of which was partially supported under this grant) [20].

The understanding we have obtained of the FDTD method has provided a complete quantification of the way in which plane waves propagate in the discrete FDTD world. Using this knowledge we were able to construct an enhancement to the total-field/scattered-field boundary, which is a boundary used to introduce field into the FDTD grid. This enhancement, which is nominally exact, can provide an enormous improvement over the traditional implementation (better than a 100 dB reduction in errors in many situations). This work is described in a paper published in *IEEE Transactions on Antennas and Propagation* [21]. Additionally Prof. Taflove invited the PI to contribute a section to the 2005 edition of his FDTD book [22] which has come to be regarded as the authoritative source for FDTD-related information.

Throughout the grant period we maintained a Web site, www.fdtd.org, that seeks to list all archival publications related to the FDTD method. This site solicits input, in the form of comments posted about work appearing in the archival literature, from the entire community interested in the FDTD method (whether applied to acoustics, electromagnetics, or solid mechanics). We have also made code available there which can be used to solve various propagation problems.

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